Submission in Response to NSF CI 2030 Request for Information

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Research Domain, discipline, and sub-discipline

Theoretical and Computational Chemistry

Title of Submission

Heterogeneous and Photochemical Catalysis

Abstract (maximum ~200 words).

The computational study of heterogeneous catalysis requires the incorporation of the catalyst itself, the host of the catalyst (typically a solid or a nanostructure), the reactants and the solvent. Such systems comprise tens of thousands to hundreds of thousands of atoms. Therefore, in order to study heterogeneous catalysis at a reliable level of accuracy requires major breakthroughs in methodology and high performance computing strategies. Photochemical catalysis presents an even greater challenge since one needs a way to address catalysis in excited electronic states. Multiple excited states are likely to be involved and therefore, surface crossings and conical intersections. New methodologies must be developed that can solve such complex problems and are also amenable to high performance computing.

Question 1 Research Challenge(s) (maximum ~1200 words): Describe current or emerging science or engineering research challenge(s), providing context in terms of recent research activities and standing questions in the field.

Heterogeneous catalysis is important for a wide variety of applications, including catalytic converters, and the conversion of various molecules to fuels. Heterogeneous catalysis is not new, but the sophistication of the experiments has increased dramatically in recent years. The computational study of heterogeneous catalysis is complicated by the very large numbers of atoms and electrons that are involved and by the need for accuracy in the computations. Consider, for example, a mesoporous silica nanoparticle or a zeolite. The computations must include the nano pore itself, catalytic groups, reactants and a solvent. This means that the calculations need to include tens of thousands to hundreds of thousands or more atoms. Common quantum chemistry methods scale on the order of N**5 to N**7, so the application of such methods to heterogeneous catalysis (or photochemical catalysis) is essentially impossible unless novel new methods are developed that can take advantage of massively parallel computers

Question 2 Cyberinfrastructure Needed to Address the Research Challenge(s) (maximum ~1200 words): Describe any limitations or absence of existing cyberinfrastructure, and/or specific technical advancements in cyberinfrastructure (e.g. advanced computing, data infrastructure, software infrastructure, applications, networking, cybersecurity), that must be addressed to accomplish the identified research challenge(s).

In order to perform calculations of the scope discussed above, one needs to develop both architectures that have petascale to exascale capability and software that can take advantage of these architectures. AZ major bottleneck is that the energy consumed by most supercomputers costs more than the hardware. So, the availability of low power computer solutions, such as graphical processing units GPUs), ARM boards and field programmable gate arrays (FPGAs). The problem one faces with these novel architectures is that low power can also mean longer time to solutions. The old tradeoff used to be accuracy vs. computational efficiency. The new tradeoff is power consumption vs. computational efficiency. An additional complication is that some of the novel architectures are difficult to program for. Electronic structure codes are varied and complex, so a large investment of people time is required to take advantage of these architectures. Few academic research groups have the required capability or interest.

Question 3 Other considerations (maximum ~1200 words, optional): Any other relevant aspects, such as organization, process, learning and workforce development, access, and sustainability, that need to be addressed; or any other issues that NSF should consider.

Workforce development is a very important issue. The conventional process is for graduate students to do publishable research, publish a few papers, complete the PhD and move on, typically to a postdoc at another university or a national laboratory. The postdoc typically works the same way: do publishable research, write papers, get a nice academic position. However, the needs described in the preceding paragraphs requires serious software development, and software development does not necessarily correspond to publishable work. This means that a new mindset is required, especially at universities, regarding what constitutes academic success. Without question, the drive to develop high performance computing that is capable of solving grand challenge problems like heterogeneous catalysis and photocatalysis will not be successful unless there is also a paradigm shift in the academic reward process.

Consent Statement

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